Implementation and Validation of the KES Turbulence Model with the Discontinuous Galerkin Spectral Element Method

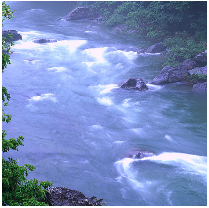
Diploma Thesis

Michael Schlottke

21st February 2012

Institut für Aerodynamik und Gasdynamik, Universität Stuttgart
Advisors: Prof. C.-D. Munz, Dr. G. Gassner, A. Beck

Turbulence simulation needs vast computational resources



- Turbulent flow is everyday phenomenon: blood flow, cloud movements, ocean currents, pipe flow, heating/cooling tasks. . .
- Accurate simulation very expensive due to large number of scales
  - Reynolds number Re characterizes level of turbulence (inertial vs. viscous forces)
  - 3D: number of operations $\sim \mathrm{Re}^{11/4}$
  - Largest direct simulations to date at Re of $\mathcal{O}(10^3)$, typical applications easily $\mathcal{O}(10^6)$ $\rightarrow$ turbulence modeling required
- Goal: combine large-eddy simulation (LES) turbulence model with high-order discontinuous Galerkin (DG) scheme

Overall approach

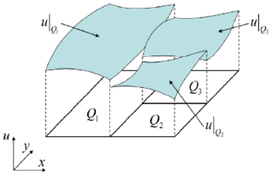
Turbulence Modeling

1. Navier-Stokes (NS) equations in conservative form
2. Apply spatial filter to yield filtered NS equations with additional unclosed terms
3. Two additional PDEs are solved for Kinetic Eddy Simulation (KES) model to calculate unclosed terms

Numerical Methods

4. Spatial discretization using the Discontinuous Galerkin Spectral Element Method (DGSEM) yields time derivative
5. Integration in time using 4th order Runge-Kutta scheme

Discontinuous Galerkin Spectral Element Method

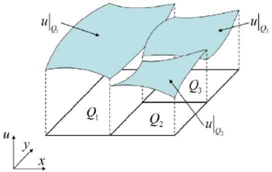


- Computational domain separated into hexahedral grid cells Q
- Starting point is weak formulation of governing equations:

$$\underline{u}_t + \nabla \cdot \underline{f} = 0 \quad \rightarrow \quad \int_Q (\underline{u}_t + \nabla \cdot \underline{f})\phi \, \mathrm{d}\underline{x} = 0$$

- Polynomial ansatz function used to approximate solution in each cell (basis functions same as test function $\rightarrow$ Galerkin)
- On cell boundaries, function values do not have to match (discontinuous), instead numerical fluxes are used

Discontinuous Galerkin Spectral Element Method



- Exact integrals in weak formulation approximated by Gauss quadrature
- Explicit operator $\partial \underline{u}_h / \partial t = \mathcal{L}_h(\underline{u}_h, t)$ integrated in time
- Advantages over FV/FEM:
  - Extremely efficient through co-location and hexahedral structure (1D $\rightarrow$ 3D: $\mathcal{O}(N) \rightarrow \mathcal{O}(3N)$ operations)
  - Higher order means higher accuracy (fewer grid points needed)
  - Very compact (exchange only cell surface data)

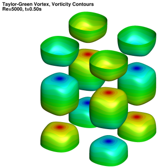
3D Taylor-Green vortex flow as challenging test case

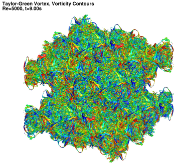
Reference problem: Taylor-Green vortex

- Laminar-turbulent transition on cube with dimensions $[2\pi]^3$
- Simple large-scale ICs, periodic BCs
- No energy source $\rightarrow$ decaying turbulence
- Number of scales controlled by $\mathrm{Re} = \frac{1}{\mu_0}$

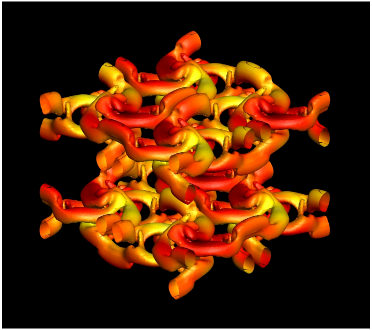
Resolution

- Calculations on structured Cartesian grid
- 8^3 grid cells, polynomial degree $N = 7$ $\rightarrow 64^3$ DOFs
- $\mathrm{Re} = 200 - 1600$

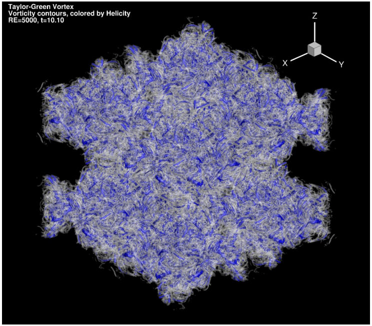




Video comparison of TGV at $\mathrm{Re} = 200$ and $\mathrm{Re} = 5000$



(a) $\mathrm{Re} = 200$, $N = 5, 96^3$ DOFs



(b) $\mathrm{Re} = 5000$, $N = 5, 600^3$ DOFs

DNS solution using Navier-Stokes. Vorticity ($\nabla \times \underline{u}$) contours, colored by helicity ($\underline{u} \cdot (\nabla \times \underline{u})$).

More stability than Navier-Stokes solution

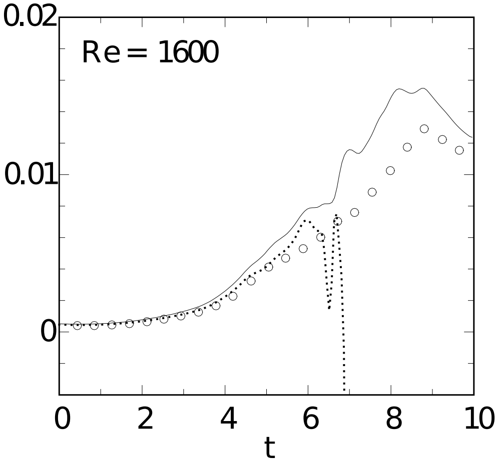


Figure: Kinetic energy dissipation rates at $\mathrm{Re} = 1600$; KES (——), Navier-Stokes ($\cdots$), DNS ($\circ$)

Very good results compared to other LES models

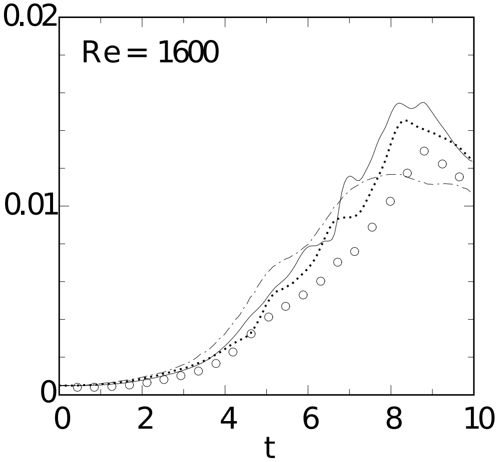


Figure: Kinetic energy dissipation rates at $\mathrm{Re} = 1600$; KES (——), ALDM (· · ·), dynamic Smagorinsky (– ·), DNS (∘)

DGSEM + KES: difficult union, but promising results

- Major difficulties:
  - Severe stability problems
  - Unusually large increase in computational time
- Upsides:
  - First successful combination of DGSEM approach with two-equation LES model
  - Preliminary results already show good performance in comparison to pure NSE and other LES models
  - No optimization of code (yet)

Next focus on improving stability, increasing efficiency, and parameter tuning

- Further stabilization through de-aliasing and filtering
- Code optimization to reduce computational time
- Adaptation of model parameters may improve accuracy
- Include higher Re cases

Backup

Spatial filtering applied to separate subgrid-scale properties

Filtering

- Spatial filtering $\Phi = \bar{\Phi} + \Phi''$ creates additional unclosed terms
- Only velocity, energy: $\tilde{\Phi} = \overline{\rho\Phi}/\bar{\rho}$ (Favre averaging)

Filtered Navier-Stokes equations

$$\text{Mass:} \quad \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i) = 0 \tag{1}$$

$$\text{Momentum:} \quad \frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_i\tilde{u}_j + \bar{p}\delta_{ij} - \tilde{\tau}_{ij} - \tau_{ij}^{\mathrm{sgs}}\right] = 0 \tag{2}$$

$$\text{Energy:} \quad \frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \frac{\partial}{\partial x_j}\Big[(\bar{\rho}\tilde{e} + \bar{p})\tilde{u}_j - \tilde{\tau}_{ij}\tilde{u}_i + \tilde{q}_j + e_j^{\mathrm{sgs}} + p_j^{\mathrm{sgs}} + \sigma_j^{\mathrm{sgs}} + q_j^{\mathrm{sgs}}\Big] = 0 \tag{3}$$

Unclosed terms determined using KES model

- KES model by Fang and Menon[1] uses eddy viscosity approach
- Unclosed terms are modeled as $f(\nu_t, \tilde{\Phi})$
- $\nu_t = C_\nu \sqrt{k^{sgs}} l^{sgs}$, C_ν: eddy viscosity parameter
- Two additional equations for k^{sgs}, l^{sgs}:

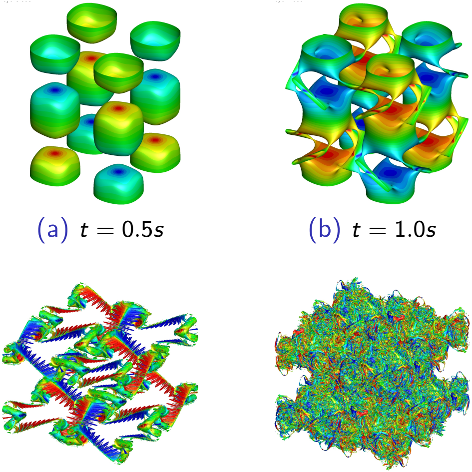
$$\frac{\partial \bar{\rho} k^{sgs}}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_j k^{sgs} - \left(\frac{\mu}{Pr} + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k^{sgs}}{\partial x_j}\right] = \tau_{ij}^{sgs}\frac{\partial \tilde{u}_i}{\partial x_j} - C_{\epsilon,k}\bar{\rho}\frac{(k^{sgs})^{3/2}}{l^{sgs}} \tag{4}$$

$$\frac{\partial \bar{\rho}(kl)^{sgs}}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_j (kl)^{sgs} - \left(\frac{\mu}{Pr} + \frac{\mu_t}{\sigma_{kl}}\right)\frac{\partial (kl)^{sgs}}{\partial x_j}\right] = C_l l^{sgs}\tau_{ij}^{sgs}\frac{\partial \tilde{u}_i}{\partial x_j} - C_{\epsilon,kl}\bar{\rho}(k^{sgs})^{3/2} \tag{5}$$

$\Rightarrow$ in total: seven PDEs to solve simultaneously

[1] Y. Fang and S. Menon: A Two-Equation Subgrid Model for Large-Eddy Simulation of High Reynolds Number Flows. 44h AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 9-12, 2006, AIAA-2006-0116.

Development of TGV solution ($Re = 5000$)



(a) $t = 0.5s$ (b) $t = 1.0s$

(c) $t = 5.0s$ (d) $t = 9.1s$

Weak formulation is basis for DG approach

- Example: use scalar conservation law-type equation
- Multiply with test function $\phi(\underline{x})$ to obtain weak formulation

$$u_t + \nabla \cdot \underline{f}(u) = 0 \quad \rightarrow \quad \int_Q (u_t + \nabla \cdot \underline{f}(u))\phi \, \mathrm{d}\underline{x} = 0$$

- Integrate over domain (cell) Q, using integration by parts and divergence theorem:

$$\int_Q u_t \phi \, \mathrm{d}\underline{x} + \oint_{\partial Q} \underline{f} \cdot \underline{n} \phi \, \mathrm{ds} - \int_Q \underline{f} \cdot \nabla \phi \, \mathrm{d}\underline{x} = 0$$

- Insert polynomial ansatz function $u\big|_G \approx u^Q = \sum_{j=1}^{n_b} a_j^Q(t)\phi_j^Q(\underline{x})$
- Replace surface integral with numerical flux g (discontinuous):

$$\int_Q u_t^Q \phi_i^Q \, \mathrm{d}\underline{x} + \oint_{\partial Q} g(u^+, u^-)\phi_i^Q \, \mathrm{ds} - \int_Q \underline{f}(u^Q) \cdot \nabla \phi_i^Q \, \mathrm{d}\underline{x} = 0$$

Strong scaling up to 131,072 processors (JUGENE)

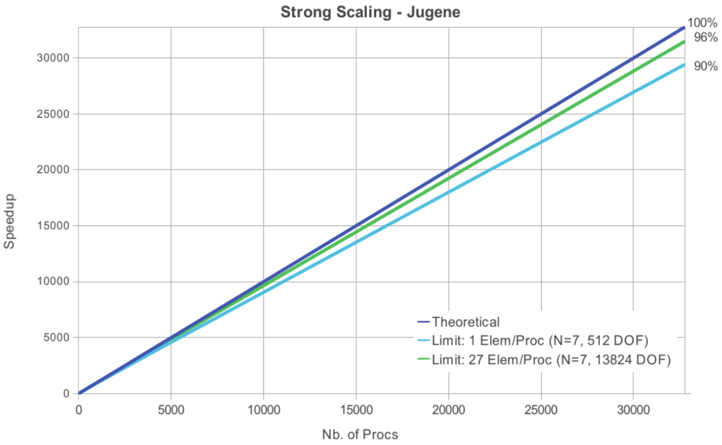


Figure: Up to 32k procs

Strong scaling up to 131,072 processors (JUGENE)

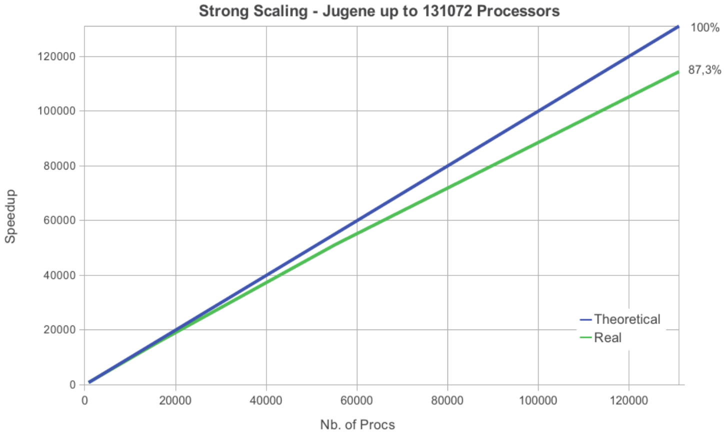


Figure: Up to 131k procs